A Novel Quasi-One-Dimensional Topological Insulator in Bismuth Iodide $\beta$-Bi$_4$I$_4$: Theoretical Prediction and Experimental Confirmation

OLEG V. YAZYEV, GABRIEL AUTES, EPFL, ANNA ISAEVA, TU Dresden, LUCA MORESCHINI, LBNL, JENS C. JOHANNSEN, ANDREA PISONI, EPFL, TAISSIA G. FILATOVA, ALEXEY N. KUZNETSOV, MSU, LÁSZLÓ FORRÓ, EPFL, WOUTER VAN DEN BROEK, Ulm University, YEONGKWAN KIM, JONATHAN D. DENLINGER, ELI ROTENBERG, AARON BOSTWICK, LBNL, MARCO GRIONI, EPFL — A new strong $Z_2$ topological insulator is theoretically predicted and experimentally confirmed in the $\beta$-phase of quasi-one-dimensional bismuth iodide Bi$_4$I$_4$. According to our first-principles calculations the material is characterized by $Z_2$ invariants $(1;110)$ making it the first representative of this topological class. Importantly, the electronic structure of $\beta$-Bi$_4$I$_4$ is in proximity with both the weak topological insulator phase $(0;001)$ and the trivial phase $(0;000)$, suggesting that a high degree of control over the topological electronic properties of this material can be achieved. Experimentally produced samples of this material appears to be practically defect-free, which results in a low concentration of intrinsic charge carriers. By using angle-resolved photoemission spectroscopy (ARPES) on the $(001)$ surface we confirm the theoretical predictions of a highly anisotropic band structure with a small band gap hosting topological surface states centered at the $\bar{M}$ point, at the boundary of the surface Brillouin zone.

$^1$We acknowledge support from Swiss NSF, ERC project “TopoMat”, NCCR-MARVEL, DFG and US DoE. G.A., A.I., L.M. and J.C.J. contributed equally to this work.

Oleg Yazyev
EPFL

Date submitted: 13 Nov 2014
Electronic form version 1.4